

# Multi-quantum eigenstates of a linear chain of coupled qubits

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We present a technique to identify exact analytic expressions for the multi-quantum eigenstates of a linear chain of coupled qubits. A choice of Hilbert subspaces is described which allows an exact solution of the stationary Schrödinger equation without imposing periodic boundary conditions and without neglecting end effects, fully including the dipole-dipole nearest-neighbor interaction between the atoms. The treatment is valid for an arbitrary coherent excitation in the atomic system, any number of atoms, any size of the chain relative to the resonant wavelength and arbitrary initial conditions of the atomic system. The procedure we develop is general enough to be adopted for the study of excitation in an arbitrary array of atoms including spin chains and one-dimensional Bose-Einstein condensates.

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It is well established that a large scale quantum computation will require a large number of strongly coupled atoms (qubits) and in particular multi-photon excitations to create large quantum superpositions of different quantum states of the system [1]. Naturally, this means that an operation of such systems will require collective excitations involving more than one photon. Although collective excitations in multi-atom systems have been studied in the past, it was typically done in the context of radiation properties of a large number of atoms randomly distributed in space, such as in a gas cell [2]. There have been many exact studies of collective eigenstates of spatially ordered systems, such as Heisenberg chains [3, 4, 5]. However, these studies suffer from one common drawback: they are limited to finding the ground state or one-photon excited states in the limit of a large number of atoms, or are subject to periodic boundary conditions.

With the recent progress in trapping and cooling of a small number of atoms or ions, the attention has been drawn towards systems that are comprised of a small number of atoms having a definite geometrical arrangement, as dictated by the confining field of a hypothetical atom trap [6]. A number of analytical studies have been performed on systems composed of  $N$  atoms confined to fixed positions, with a particular interest in ring arrangements [7], perhaps as they have periodic boundary conditions which makes the eigenstates easier to obtain. However, exact analytic studies, which give explicit forms of the eigenstates, have been performed on systems containing only two and three atoms [7, 8, 9]. More general results valid for arbitrary  $N$  have also been given [10, 11], but are limited to one-photon excitations only. More exotic shapes, such as diamond structures [12], have also been investigated, but the calculations were limited to two-photon excitations and small numbers of atoms. While these schemes successfully demonstrate the situation for obtaining one- or two-photon-excited states in  $N$ -atom systems, the analysis for the excitation of such a system by an arbitrary number of photons, giving a multi-quantum eigenstate, is unknown.

Other treatments of these systems stem from statistical physics, where properties are extracted from the partition function, which is determined by the eigenvalues of the system. The partition function can provide a witness to entanglement [13], it does not, however, give information about the energy eigenstates of the system. These states may have applications in quantum information and need to be quantified in order to perform quantum computation. This forms the motivation of this work to derive the explicit analytic expressions for the multi-quantum eigenstates of a linear chain of  $N$  atoms that can be applied to a variety of settings. The availability of these eigenstates is highly advantageous because it provides a convenient ground for rigorous examination of entangled properties of a particular arrangement of atoms and facilitates the explicit study of the stability of entangled states, something which can be obscured if we remove this generality. It may also provide an interesting tool to study entanglement creation in 1D Bose-Einstein condensates [14]. We cover the case of the linear chain as although it is one of the simplest structures that can be constructed in an atom trap, it has not been solved exactly while imposing the generality that we demand here. There is also a considerable interest in analyzing multi-atom systems to realize a phase gate operation [15], in which we do not impose periodic boundary conditions and include the end effects.

In this paper, we study the creation of multi-quantum eigenstates in a linear chain of  $N$  identical, equally spaced and confined to fixed positions, two-level atoms each interacting only with its nearest neighbors through the dipole-dipole interaction. This model might be realized in practice by placing the atoms in a tightly confining linear trap, an optical lattice or in an atomic chip [16, 17]. The Hamiltonian for the linear chain of atoms is given by

$$\hat{H} = \hat{H}_0 + \hat{V} = \hbar\omega_0 \sum_{i=1}^N \hat{S}_i^z + \hbar\Omega \sum_{\substack{i,j=1 \\ |i-j|=1}}^N \hat{S}_i^+ \hat{S}_j^-, \quad (1)$$

where  $\hat{H}_0$  is the interaction-free Hamiltonian and  $\hat{V}$  is the dipole-dipole interaction between the atoms.

In Eq. (1),  $\omega_0$  is the transition frequency of a two-level atom in isolation,  $\hat{S}_i^z$  is the energy operator of the  $i$ -th atom, and  $\hat{S}_i^+$ ,  $\hat{S}_i^-$  are the raising and lowering operators for the  $i$ -th atom, respectively. The dipole-dipole interaction parameter  $\Omega \equiv \Omega(r_{ij})$  depends on the distance  $r_{ij}$  between adjacent atoms in the linear chain and the polarization of the atomic dipole moments relatively to the interatomic axis [2].

To find the multi-quantum energy states of the system, we have to solve the stationary Schrödinger equation with the Hamiltonian  $\hat{H}$ . We propose a procedure which, despite of the complexity of the problem, facilitates an exact analytic solution of the Schrödinger equation valid for an arbitrary number of excitations  $M$ . The interaction-free Hamiltonian  $\hat{H}_0$  has  $N + 1$  energy levels of energies  $E_0^{(M)} = M\hbar\omega_0$ , where  $M = 0, 1, 2, \dots, N$ . Since there are  $N$  two-level atoms, it follows that  $\hat{H}_0$  operates on a  $2^N$ -dimensional Hilbert space  $W$ . We can index the atoms in the chain by the numbers 1 to  $N$ ; collective excitations the system can then be represented using the ket  $|k_1, \dots, k_M\rangle$ , where the non-zero integers  $k_1, \dots, k_M$  denote the indices of the atoms which are in their excited state:

$$|k_1, \dots, k_M\rangle = \hat{S}_{k_1}^+ \dots \hat{S}_{k_M}^+ |0\rangle, \quad (2)$$

where  $|0\rangle$  denotes the ground state of the collective system, and is nondegenerate. The ground states  $|0\rangle$  and excited states  $|k_1, \dots, k_M\rangle$  form a basis which spans  $W$ . The maximally excited interaction-free energy eigenstate, i.e. the collective state where all  $N$  atoms are in their upper state, is then represented by  $|1, 2, \dots, N\rangle$  in our notation.

Under the action of  $\hat{H}_0$ , a particular energy level  $M$  has a degeneracy factor of  $N!/(N - M)!M!$ , which is equal to the number of ways  $N$  atoms can be divided into two groups, with  $M$  atoms excited and  $N - M$  atoms in their ground states. However, while  $\hat{H}$  acts on the same Hilbert space  $W$ , it leads to a significant splitting of the degeneracies of the collective system.

We observe that the process of finding the eigenstates of  $\hat{H}$  may be simplified by noting that  $\hat{H}_0$  and  $\hat{V}$  commute. Since

$$\frac{[\hat{H}_0, \hat{V}]}{\omega_0 \Omega \hbar^2} = \sum_{\substack{i, j, k=1 \\ |j-k|=1}}^N (S_j^+ [S_i^z, S_k^-] + [S_i^z, S_j^+] S_k^-), \quad (3)$$

and using the relations  $[S_i^z, S_j^\pm] = \pm S_i^\pm \delta_{ij}$ , we can easily see that  $[\hat{H}_0, \hat{V}] = 0$ . This result, coupled with the fact that  $\hat{H}_0$  and  $\hat{V}$  are Hermitian means that the operators  $\hat{H}_0$  and  $\hat{V}$  share a complete set of orthonormal eigenstates  $\{|\phi_i\rangle\}$ . Since  $\hat{H}$  is just the sum of these two operators, and  $\{|\phi_i\rangle\}$  is a complete set, it follows that  $\hat{H}$ ,  $\hat{H}_0$  and  $\hat{V}$  share the same complete set of orthonormal eigenstates

$\{|\phi_i\rangle\}$ . The  $\hat{H}_0$  operator allows us to partition the state vector space  $W$  into  $N + 1$  subspaces  $W^j$ :

$$W = \bigoplus_{j=0}^N W^j, \quad (4)$$

where the subspace  $W^j$  corresponds to all states which give an eigenvalue of  $j\hbar\omega$  when operated on by  $\hat{H}_0$ , and is of dimensionality  $N!/(N - j)!j!$ . In this way, we see that  $\hat{H}_0$  is an automorphism  $T(\hat{H}_0) : W^j \rightarrow W^j$  for all  $W^j$ . Since  $\hat{H}$  and  $\hat{V}$  commute with  $\hat{H}_0$ , they must be mappings of the form  $W^j \rightarrow W^j$  for all subspaces  $W^j$ . Thus, to find the energy eigenstates of the system, we can solve the Schrödinger equation for  $\hat{H}$  for each subspace  $W^j$  instead of  $W$ . However, all states in a particular  $W^j$  are eigenstates of  $\hat{H}_0$ , so we can neglect this operator and simply solve the Schrödinger equation for  $\hat{V}$ . To accomplish this, we take the most general state vector one can form in the subspace  $W^M$ :

$$|\psi^{(M)}\rangle = \sum_{k_1 < \dots < k_M} C(k_1, \dots, k_M) |k_1, \dots, k_M\rangle, \quad (5)$$

where the summation runs through all  $M$ -tuples  $(k_1, \dots, k_M)$  such that  $1 \leq k_1 < \dots < k_M \leq M$ . To then obtain the energy eigenstates, we solve

$$\hat{V}|\psi^{(M)}\rangle = \Delta E |\psi^{(M)}\rangle, \quad (6)$$

where  $|\psi^{(M)}\rangle \in W^M$  and  $\Delta E$  is the energy level shift associated with the dipole-dipole interaction  $\hat{V}$ . The eigenvalue associated with  $\hat{H}$  is then given by

$$\begin{aligned} \hat{H}|\psi^{(M)}\rangle &= \hat{H}_0|\psi^{(M)}\rangle + \hat{V}|\psi^{(M)}\rangle \\ &= (E_0^{(M)} + \Delta E)|\psi^{(M)}\rangle. \end{aligned} \quad (7)$$

We assume that the energy eigenstates of the interaction Hamiltonian are of the form (5) and constitute a complete set. In order to determine the coefficients  $C(k_1, \dots, k_M)$ , we substitute (5) into Eq. (6), and find the following multi-term recurrence relation relating the coefficients  $C(k_1, \dots, k_M)$  to the energy eigenvalue shift  $\Delta E$ :

$$\begin{aligned} \Delta E C(k_1, \dots, k_M) &= \hbar\Omega \sum_{j=1}^M [C(k_1, \dots, k_j + 1, \dots, k_M) \\ &\quad + C(k_1, \dots, k_j - 1, \dots, k_M)], \end{aligned} \quad (8)$$

where it is assumed that the summation in the above expression must not include terms which have an invalid value for  $k_j$ , i.e. are not generated by Eq. (6). There are only three such cases: (a) when  $k_1$  is equal to zero or (b)  $k_M = N + 1$  and thus the index cannot refer to an actual atom, and (c) when two of the  $k_j$  are equal, which would rule out the state from being an eigenvector of  $\hat{V}$ .

Equation (8) without such a restriction on summation can be solved easily, so we prescribe the following

method: we allow invalid terms to be included in Eq. (8), on the condition that they must vanish. This means that we now regard cases (a), (b), and (c) as conditions under which a coefficient must vanish.

By inspection, we see that Eq. (8) resembles a pattern that is seen in sine or cosine functions  $f(x)$ , for  $f(x+1) + f(x-1) \propto f(x)$ . As a trial solution, we thus consider the general form

$$C(k_1, \dots, k_M) = \sum_{a, \dots, d} K_{a \dots d} f_a(\alpha_a k_1 + A_a) \dots f_d(\delta_d k_M + D_d), \quad (9)$$

where  $\alpha_a, \dots, \delta_d$  and  $A_a, \dots, D_d$  are arbitrary constants along with  $K_{a \dots d}$ , and the summation range for the  $M$  indices  $a, \dots, d$  ranges from 1 to  $M$ . By operating on the  $k_j$  individually by sine or cosine functions, this expansion can be made fully consistent with Eq. (8) using further restrictions which now follow.

The only way that condition (c) can be satisfied is if  $K_{a \dots d}$  is antisymmetric in any two pairs of indices. Condition (a) then implies that either all the  $f_i$  are sine functions with the offsets  $A_i, \dots, D_d$  equal to zero or the  $f_i$  are cosine functions where  $A_i, \dots, D_d$  are all equal to  $\pi/2$ . These solutions are not independent – they are equal up to a multiplicative constant, so we choose the sine function. The antisymmetry property also requires that  $\alpha_i = \dots = \delta_i$ . We then have

$$C(k_1, \dots, k_M) = K \epsilon_{a \dots d} \sin(\alpha_a k_1) \dots \sin(\alpha_d k_M), \quad (10)$$

where  $\epsilon_{a \dots d}$  is the permutation (Levi-Civita) symbol and summation is implied over the repeated  $M$  symbols  $a, \dots, d$  from 1 to  $M$ . The constant  $K$  will be set equal to unity from now on as it is not constrained by any conditions.

For condition (b) to be satisfied, and owing to the permutations of the  $\alpha_i$ , the constants  $\alpha_1, \dots, \alpha_M$  must equal  $g_1 \theta, \dots, g_M \theta$ , where  $\theta = \pi/(N+1)$  and the  $g_i$  are integers. Our solution now becomes

$$C(k_1, \dots, k_M) = \epsilon_{a \dots d} \sin(g_a k_1 \theta) \dots \sin(g_d k_M \theta), \quad (11)$$

or equivalently

$$C(k_1, \dots, k_M) = \epsilon_{a \dots d} \sin(g_1 k_a \theta) \dots \sin(g_M k_d \theta). \quad (12)$$

We have thus derived the coefficients apart from the arbitrary integers  $g_1, \dots, g_M$ . Clearly, no two  $g_i$  can be equal, for the  $C(k_1, \dots, k_M)$  would vanish due to the presence of the permutation symbol. Also, to avoid duplicate cases, we require for non-trivial eigenstates that

$$g_1 < \dots < g_M. \quad (13)$$

If a particular  $g_i$  is equal to  $N+1$ , the coefficient  $C(k_1, \dots, k_M)$  vanishes; therefore all the  $g_i$  must be less than or greater than  $N+1$ . The difference between these two cases amounts to multiplying Eq. (12) by a minus

sign on the right-hand side. Since such a factor is irrelevant, we impose the restriction that  $g_i \leq N$  for all  $g_i$ . Due to the properties of the sine function, this implies also that  $g_i \geq 1$  for all  $g_i$ . Thus we can state constraints on the  $g_i$ :

$$1 \leq g_1 < \dots < g_M \leq N. \quad (14)$$

Now that we have determined the coefficients of the eigenstates (5), we are in a position to determine the energy eigenvalue shift. Using (8), we have

$$\begin{aligned} \Delta EC(k_1, \dots, k_M) &= \hbar \Omega \sum_{j=1}^M 2 \cos(g_c \theta) [\epsilon_{a \dots c \dots e} \sin(g_a k_1 \theta) \dots \\ &\dots \sin(g_c k_j \theta) \dots \sin(g_e k_M \theta)], \end{aligned} \quad (15)$$

where we have converted pairs of terms of the form  $\sin g_c(k_j + 1)\theta$  and  $\sin g_c(k_j - 1)\theta$  into the product  $2 \cos g_c \theta \sin g_c k_j \theta$ . We repeat this for each sine pair, giving the end result

$$\begin{aligned} \Delta EC(k_1, \dots, k_M) &= 2 \hbar \Omega C(k_1, \dots, k_M) \\ &\times \sum_{i=1}^M \cos(g_i \theta). \end{aligned} \quad (16)$$

The energy eigenvalue shift is thus given by

$$\Delta E = 2 \hbar \Omega \sum_{i=1}^M \cos(g_i \theta). \quad (17)$$

We now collect the results to give the energy eigenstates and eigenvalues for the system (1), valid for an arbitrary number of atoms  $N$  and an arbitrary number of excitations  $M$ . The unnormalized energy eigenstates of (1) are given by

$$|\psi_{g_1 \dots g_M}^{(M)}\rangle = \sum_{k_1 < \dots < k_M} C_{g_1 \dots g_M}^{k_1 \dots k_M} |k_1, \dots, k_M\rangle, \quad (18)$$

with corresponding eigenvalues

$$E_{g_1 \dots g_M}^{(M)} = M \hbar \omega_0 + 2 \hbar \Omega \sum_{i=1}^M \cos(g_i \theta) \quad (19)$$

where

$$C_{g_1 \dots g_M}^{k_1 \dots k_M} = \epsilon_{a \dots d} \sin(g_a k_1 \theta) \dots \sin(g_d k_M \theta), \quad (20)$$

and  $\theta = \pi/(N+1)$ . The parameter  $M$  equals the number of excited atoms in a particular eigenstate, and thus forms one of the quantum numbers that enumerate the energy eigenstates. The other quantum numbers are the  $M$  numbers  $g_i$ , which are subject to the constraint (14). There are  $N!/(N-M)!$  ways of choosing values for the  $g_i$  so that for all  $g_i$ ,  $1 \leq g_i \leq N$ . However, the constraint (14) forces us to divide the number of combinations by the number of ways one can re-label the  $g_i$ , which

is  $M!$ . Hence there are  $N!/(N - M)!M!$  energy eigenstates associated with a given value of  $M$ . Note that the number of the states for a given  $M$  is the same as it was in the interaction-free system mentioned earlier.

To fit the ground eigenstate ( $M = 0$ ) into the solution (18), we observe that  $C_{g_1 \dots g_M}^{k_1 \dots k_M}$  has no  $g_i$ 's and no  $k_j$ 's for the case  $M = 0$ , so we define  $C_{g_1 \dots g_M}^{k_1 \dots k_M} = C$ , an arbitrary constant which may be set equal to unity. Clearly the summation sign in (18) disappears in this case, and the only ket present is defined to be that corresponding to the ground state of the system,  $|0\rangle$ .

One can see the step which enabled us to determine the exact analytic expressions for the multi-quantum eigenstates. The recurrence relation derived from the eigenvalue equation had restrictions on its summation range; however, it is clear that there is a simple pattern in the summation formula. We completed the pattern by including invalid terms, and created boundary conditions which made these extra terms vanish. Other treatments handle the problem of the restrictions on the original summation by imposing periodic boundary conditions. However, the latter treatment implicitly converts the linear chain into a ring – a different physical system. That the derived states are eigenstates of a linear chain Hamiltonian is the justification of our approach.

As an illustration of our general solution, we discuss two specific examples,  $M = 1$  and  $M = 2$ , corresponding to single- and two-photon excitation of the  $N$ -atom system. The general eigenstates (18) for  $M = 1$  simplify to

$$|\psi_{g_1}^{(1)}\rangle = \sum_{k=1}^N \sin(g_1 k \theta) |k\rangle, \quad (21)$$

where  $1 \leq g_1 \leq N$  is a single quantum number differentiating between  $N$  states. The associated eigenvalues are

$$E_{g_1}^{(1)} = \hbar\omega_0 + 2\hbar\Omega \cos g_1 \theta. \quad (22)$$

For these states, we can see an interesting property in the small sample model, where the interatomic separation is much smaller than transition wavelength [18]. For the states where  $g_1$  is even, the transition dipole moment  $\langle \psi_g^{(1)} | \hat{\mu} | 0 \rangle$ , where  $|0\rangle$  is the ground state, vanishes. The reason for this is that the coefficient of  $|k\rangle$  is the negative of the coefficient of  $|N + 1 - k\rangle$  in the above eigenstate expansion for such states. The sum of these coefficients then gives zero for the transition dipole moment. Thus  $g_1$ -even states do not spontaneously decay to the ground state.

For  $M = 2$ , the eigenstates are of the form

$$|\psi_{g_1 g_2}^{(2)}\rangle = \sum_{k_1=1}^{N-1} \sum_{k_2=k_1+1}^N [\sin(g_1 k_1 \theta) \sin(g_2 k_2 \theta) - \sin(g_1 k_2 \theta) \sin(g_2 k_1 \theta)] |k_1, k_2\rangle, \quad (23)$$

with energies

$$E_{g_1 g_2}^{(2)} = 2\hbar\omega_0 + 2\hbar\Omega(\cos g_1 \theta + \cos g_2 \theta). \quad (24)$$

For this case,  $1 \leq g_1 < g_2 \leq N$ , giving a total of  $N(N - 1)/2$  eigenstates. This is the first excitation level where the antisymmetric property of the  $C_{g_1 \dots g_M}^{k_1 \dots k_M}$  appears. For a small number of atoms,  $N = 3$ , the above eigenstate and eigenvalue examples agree (apart from the normalization constant) with the case of the isosceles triangle [7] flattened into a straight line, with the dipole-dipole interaction between the two atoms at the ends of the line removed.

In summary, we have proposed a simple and robust method to derive exact expressions for the multi-quantum states of a linear chain of  $N$  trapped atoms interacting with its nearest neighbors through the dipole-dipole interaction. The method is based on a technique of converting the eigenvalue equation into a specific recurrence relation, rather than the usual technique of diagonalizing a matrix, the latter being more suited to the case where the number of atoms is not arbitrary.

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